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Romanov, Mikhail; Hansen, Per Christian; Dahl, Anders Bjorholm

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A Parameter Choice Method for Simultaneous Reconstruction and Segmentation

Mikhail Romanov, Per Christian Hansen, Anders Bjorholm Dahl

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Abstract

The problem of finding good regularization parameters for the reconstruction problems without knowledge of the ground truth is a non-trivial task. We overview the existing parameter-choice methods and present the modified L-curves approach for a good regularization parameters selection that is suited for our Simultaneous Reconstruction and Segmentation method. We verify the validity of this approach with numerical experiments based on reconstructions of artificial phantoms from noisy data, and the problems in our numerical experiments are underdetermined.

1 Introduction

In this work we consider tomographic reconstruction of an object's interior from X-ray transmission projections. The geometry of the projections is parallel-beam geometry. The amount of data is less than the amount of the pixels in image - thus, the problem is underdetermined. Also, the data is not perfect and contains some amount of noise.

To deal with this problem we formulate a minimization problem that contains three terms:

$$\lambda_1 \mathcal{D}(\mathbf{x}), \mathcal{C}(\mathbf{x}, \delta), \lambda_2 \mathcal{R}(\delta), \tag{1}$$

where $\mathbf{x}$ is the image, δ is a Hidden Markov Measure Field Model (will be explained later), $\mathcal{D}$ is a data fitting term, $\mathcal{C}$ is a class fitting term, $\mathcal{R}$ is a segmentation regularization term. To balance these terms we need two regularization parameters: λ_1, λ_2. In order to make the best reconstruction, we need to find the best regularization parameters. In this work we consider an approach that may help to find good regularization parameters.

The parameter selection is an important problem for the reconstruction process. In case the ground truth of the reconstruction is known, then the process of selection of the optimal parameters is trivial: the set of parameters are checked and after that the parameters that leads to the smallest errors are selected.

In real-world problems this task may not be trivial as the ground truth is not known. In this case the choice of the best parameters for the reconstruction algorithm is hard, and we need to use some heuristics to understand how good or how bad is the resulting reconstruction. Also, the fact that usage of these heuristics does not perform well in all cases should be accepted. In addition, each of the heuristics has its own limitations. In some cases one of the heuristics will perform very well, in other cases it will fail.

In this work we will make our proposal for a good heuristic that will lead to a good choice of the regularization parameters for the Simultaneous Reconstruction and Segmentation Algorithm (SRS) [17].

The main idea of the SRS algorithm is to compute a reconstruction with a segmentation (i.e. the different materials locations) in a joint fasion. The information about the materials is given beforehand. We use this information to make the reconstructions and segmentation more precise than what is possible to do in a classical, non-simultaneous way. The SRS algorithm is a variational algorithm, the minimization problem has three terms and two regularization parameters.

There is a bunch of well-known techniques to choose the regularization parameter. One approach to solve this problem is the discrepancy principle (DP) [11][1][16]. The main idea of this method is that the discrepancy between the measured data and the data predicted by the reconstructed image should be comparable to the standard deviation of the noise. In case the discrepancy is bigger then the standard deviation of noise, that means that the solution may be computed better. In case it is smaller, then there is high risk of overfitting the noise. This approach is applicable to problems with Gaussian noise. In case the noise is different from Gaussian, then the estimation of discrepancy may be a tough problem. Besides, the amount of noise needs to be known. This also causes some limitations.

A modification of the previous method that generalizes the approach and makes it possible to use it without knowing the exact level of the noise is called the L-curve method [3][7][5]. The main idea of this approach is that a good regularization parameter represents a good balance between the data fit and the regularization. This good compromise is usually seen on the plot of the regularization term plotted versus the data fitting term and represented by a corner of the graph.

Another important method is Generalized Cross-Validation (GCV) [2][14][10]. The main idea of cross validation is that reconstruction of the image is done from incomplete data, where one of the instances is left out, and then we compute the estimated value of the left out instance from the image reconstruction. In principle we do this procedure for each of the data instances and the regularization parameter is chosen such that the prediction errors are minimized. GCV is another method for doing this. Instead of doing the reconstruction for leaving out each of the data points, one may do only one reconstruction for each of regularization parameters and then to compute the residual norm normalized by a factor that takes into account the reduction of the amount of degrees of freedom the measurement geometry. The objective is to find the regularization parameters that minimize this normalized sum of the errors. This method is one of the most efficient ones, but it has a significant drawback: defining and computing the denominator for the GCV function is a difficult problem, except for Tikhonov Regularization [15] and Truncated SVD [?].

One more important method of parameter selection is called Normalized Cumulative Periodogram (NCP) [13]. The idea of this method lies in the field of spectral analysis. In this approach we analyze the difference between the real data and the data predicted by the image, referred to as residual. If the solution is underregularized, the high frequencies are more represented in the residual. In case the solution is overregularized, the low frequencies will be more represented in the residual. The optimal regularization parameter, from the point of view of the NCP, represents an equal amount of high and low frequencies. The shortcoming of this approach that to use this criterion, we need to know or to be able to compute the spectrum of the problem.

More information about the regularization parameter choice methods can be found in the books [4], [6].

To sum up, we have four candidate strategies to find the optimal regularization parameters: DP, L-curve, GCV, NCP. The use of GCV is not possible as we do not know how to define the normalization coefficients in the error function. For the DP we need to know the norm of the noise that is not always known. As for the other methods, it makes sense to try them.

2 Brief Description Of the SRS Method

In this work we reconstruct the object $\mathbf{x}$ from the projections $\mathbf{b}$. The underlying problem has the form:

$$\mathbf{b} = A\mathbf{x} + \epsilon, \tag{2}$$

where ϵ is the vector of noise in each datum. In this work we assume that the noise is Gaussian and is independent in all different measurements, has zero mean and the same standard deviation in each datum. The matrix A corresponds to the projections geometry. The element of this matrix a_{ij} is the length of the ray that corresponds to the measurement i inside of the pixel j.

We want to make a reconstruction of the object's attenuation coefficients $\mathbf{x}$ from the data $\mathbf{b}$ with the assumption that the object consists of several materials, each of these materials is characterized by the mean value μ_k of the attenuation coefficient and the standard deviation σ_k of the attenuation coefficient and with Gaussian distribution of the attenuation coefficient. Thus, the attenuation coefficient has the following distribution given that it belongs to class k:

$$p(x_j|k) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x_j - \mu_k)^2}{2\sigma_k^2}\right). \tag{3}$$

The algorithm that we use for the tomographic reconstruction of the image is the Simultaneous Reconstruction and Segmentation (SRS) algorithm. This algorithm uses the concept of a Hidden Markov Measure Field Model (HMMFM) CITE as the model for the segmentation. This model assigns to each of the pixels j the probability δ_{jk} to belong to each of the possible classes k. As these values are probabilities, they sum to 1:

$$\forall j \quad \sum_k \delta_{jk} = 1. \tag{4}$$

Also, the probabilities can not be negative:

$$\forall j, k \quad \delta_{jk} \geq 0. \tag{5}$$

The problem that is solved is formulated in the following way:

$$\begin{aligned}
\min_{\mathbf{x},\delta} \quad & \lambda_1 \|A\mathbf{x} - \mathbf{b}\|_2^2 - \\
& \sum_j \log \sum_k \frac{\delta_{jk}}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x_j - \mu_k)^2}{2\sigma_k^2}\right) + \\
& \lambda_2 \sum_j \sum_{j' \in N_j} \sum_k \left(\delta_{jk} - \delta_{j'k}\right)^2 \\
\text{s.t.} \quad & \forall j \ \sum_k \delta_{jk} = 1, \\
& \forall j, k \ \delta_{jk} \geq 0.
\end{aligned} \tag{6}$$

Here x_j is the value of the attenuation coefficient inside pixel j, λ_1 and λ_2 are the regularization parameters that we would like to find, N_j is the set of neighbours of pixel j. This problem is non-convex because of the second term. In this approach we use μ_k and σ_k as a prior knowledge about the object under the reconstruction.

To solve this problem an iterative two-step approach is used. In the first stage we find the new image iterate solving the problem

$$\begin{aligned}\mathbf{x}^{l+1} = \arg\min_{\mathbf{x}} \quad & \lambda_1 \|A\mathbf{x} - \mathbf{b}\|_2^2 + \\ & \sum_j \frac{(x_j - \hat{\mu}_j)}{2\hat{\sigma}_j},\end{aligned} \tag{7}$$

where $\mathbf{x}^{l+1}$ is the $l+1$ iterate for $\mathbf{x}$, the values $\hat{\mu}_j$ and $\hat{\sigma}_j$ are the expected value of the pixel j attenuation coefficient and the standard deviation of the pixel j attenuation coefficient:

$$\tilde{\mu}_j = \sum_k \delta_{jk} \mu_k \tag{8}$$

$$\tilde{\sigma}_j^2 = \sum_k \delta_{jk} (\mu_k^2 + \sigma_k^2) - \hat{\mu}_j^2. \tag{9}$$

The substitutions (7), (8), (9) of the original image optimization problem that is part of the problem (6) makes it convex and easy to solve.

After the image has been updated, we update the HMMFM solving the problem:

$$\begin{aligned}\delta^{l+1} = \arg\min_{\delta} \quad & -\sum_j \log \sum_k \frac{\delta_{jk}}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x_j^{l+1} - \mu_k)^2}{2\sigma_k^2}\right) + \\ & + \lambda_2 (\delta_{jk} - \delta_{j'k})^2 \\ s.t.\ \forall j \quad & \sum_k \delta_{jk} = 1, \\ \forall j, k \quad & \delta_{jk} \geq 0.\end{aligned} \tag{10}$$

After the HMMFM is updated using (10), the image is recomputed again according to (7) and so forth. After the convergence of this process it is possible to add one more stage of making the image more sharp. This enhancement deals with the fact that we do not solve the original problem (6), but a simplified version of it. From our experience, this makes sense only in case the iterative process described above converges to a good approximation of the solution. Thus, we do not consider this enhancement here as the optimal parameters for this procedure should also be optimal for the procedure above.

To sum up, our aim is to find the regularization parameters for the reconstruction procedure, described by (7), (10). For more details and numerical examples, see [12].

3 Parameter Selection Algorithm

To find a good parameter selection algorithm we have modified the L-curve criterion.

The original L-curve criterion is formulated as follows: suppose we have the data fitting term $\mathcal{D}(\mathbf{x})$ (in our case this is $\|A\mathbf{x} - \mathbf{b}\|_2$) and the regularization term $\mathcal{R}(\mathbf{x})$, where both terms are convex. In this case the whole problem may be formulated as:

$$\min_{\mathbf{x}} \lambda \mathcal{D}(\mathbf{x}) + \mathcal{R}(\mathbf{x}). \tag{11}$$

Then the L-curve is defined as a log-log plot of $\mathcal{D}(\mathbf{x})$ against $\mathcal{R}(\mathbf{x})$ for different regularization parameters λ. As an example, in case the reconstruction problem is formulated as

$$\min_{\mathbf{x}} \lambda \|A\mathbf{x} - \mathbf{b}\|_2^2 + \sum_j \|D_j \mathbf{x}\|_2, \tag{12}$$

where D_j is a discrete approximation of the gradient length in the pixel j, then the L-curve is the plot of $\|A\mathbf{x}-\mathbf{b}\|_2$ against $\sum_j \|D_j\mathbf{x}\|_2$ as a function of the regularization parameters. The best regularization parameter is usually supposed to be in the corner of the L-curve that represents a balance between the data fitting term and the regularization term. In case the regularization parameter deviates to the larger side, the more emphasis is put on the data fitting term and the more is the overfitting of the noise. This corresponds to a significant growth of the regularization term $\mathcal{R}(\mathbf{x})$ and insignificant improvement of the data fitting term $\mathcal{D}(\mathbf{x})$. In case the regularization parameter is lower then the optimal one, less emphasis is put on the data fitting term and, thus, the result is overregularized. This situation corresponds to insignificant improvement of the regularization term $\mathcal{R}(\mathbf{x})$ and significant growth of the data fitting term $\mathcal{D}(\mathbf{x})$.

Our problem has a nice variational formulation and, thus, the L-curve is a good candidate for the parameter selection approach. On the other hand our problem is a non-convex problem (see (6)) and this may cause some difficulties during analysis of the L-curve. To deal with it, we need to make some modifications to the L-curve approach. Also, we have two regularization parameters. This makes the problem significantly more complicated. We also have to find a way to deal with this.

First, let us consider the task of finding a good regularization parameter λ_1 for our reconstruction problem, when λ_2 is fixed.

The λ_1 regularization parameter sets the balance in Equation (10) between the data fitting term

$$\mathcal{D}(\mathbf{x})\|A\mathbf{x}(\lambda_1,\lambda_2)-\mathbf{b}\|_2^2 \tag{13}$$

and the class fitting term

$$\mathcal{C}(\mathbf{x},\delta)-\sum_j \log \sum_k \frac{\delta_{jk}}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x_j(\lambda_1,\lambda_2)-\mu_k)^2}{2\sigma_k^2}\right). \tag{14}$$

Note that here the solution $\mathbf{x}(\lambda_1,\lambda_2)$ depends on the regularization parameters λ_1 and λ_2. The term (14) is the probability density value of the grey value x_j given the class probabilities $\delta_{j,k}$ for all k. The L-curve in this case should be represented by terms (13) and (14) values plotted against each other. We suggest to substitute the second terms' values with the values computed using the following approximation:

$$\hat{\mathcal{C}}(\mathbf{x},\delta)\sum_j \min_k \frac{(x_j-\mu_k)^2}{2\sigma_k^2}, \tag{15}$$

that corresponds to the value (14), where the actual values δ_{jk} are substituted by 1 for the class with highest probability density in the point x_j and 0 for all the other classes. The smaller the term (15), the closer the grey values of the pixels are to the means of the classes in terms of differences normalized by σ_k^{-1}. To use this approach is quite logical as the smaller is the distance of grey levels of pixels to the means of the classes, the larger is the influence of the class fitting term is. The bigger the distance the more noise in the data is overfitted.

Now, let us consider the problem of finding of good regularization parameter λ_2.

The parameter λ_2 corresponds to the balance between the last two terms in Equation (10). The first of the terms is the class fitting term (14). The second term is the HMMFM regularization term:

$$\mathcal{R}(\delta)=\sum_j \sum_k \sum_{j'\in N_j} (\delta_{jk}-\delta_{j'k})^2. \tag{16}$$

As before, the second term (14) is too complex to be analyzed. Instead of it, we will use the data fitting term (15) value for comparison.

We will present the results of this modified L-curve approach in the next section.

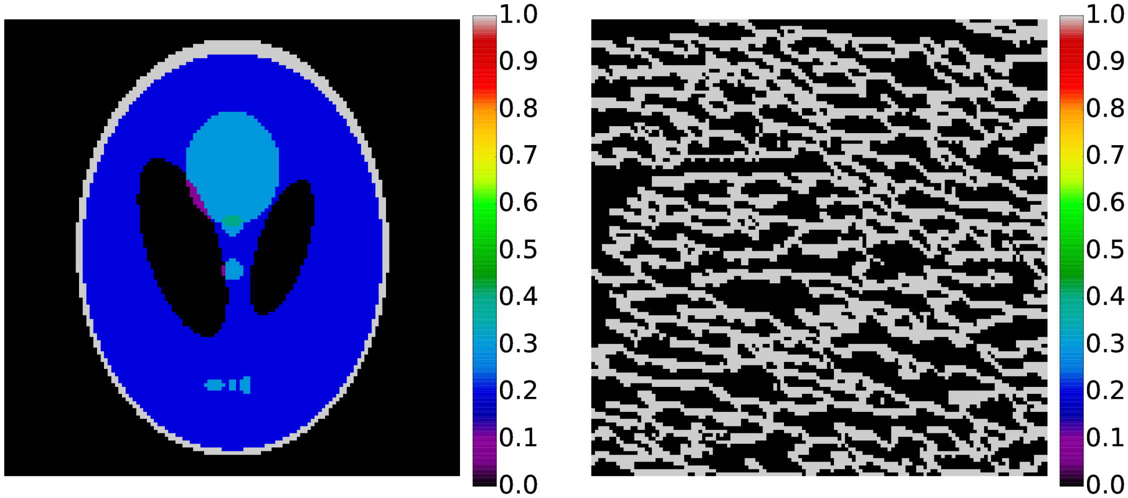

Figure 1: The phantoms that are used in the experiments. Left: Shepp-Logan phantom, generated with `MATLAB` command `phantom`, right: binary phantom, generated with command `phantomgallery` from package `AIR Tools`.

4 Results

To test our idea for choosing the regularization parameter we used two test problems. For both of these problems the artificial phantom was used as images $\mathbf{x}$. The first one was created using the standard `MATLAB` command `phantom`. Another one was the binary phantom from the `AIR Tools` package [8] and was created using the command `phantomgallery`. In both cases the phantom consists of 128×128 pixels. The phantoms are shown on Figure 1.

The first phantom has several typical attenuation coefficients: 0.0, 0.1, 0.2, 0.3, 0.4 and 1.0. The second phantom consists of only two classes of attenuation coefficients: 0.0 and 1.0.

The geometry of the projections for both problems was selected to have parallel-beam projections. The number of projections is 59, there are $\lfloor \sqrt{2} \cdot 128 \rfloor = 181$ rays in each of the projections. Thus, the ratio between amount of data and amount of pixels is equal to $\frac{\#data}{\#pixels} = 0.6$. Thus, all the problems are underdetermined. The projection matrix A was generated using the package `AIR Tools` using the function `paralleltomo`.

For both problems the data was computed according to the rule

$$\mathbf{b} = A\mathbf{x} + \varepsilon, \tag{17}$$

where for both problems ε is the different for each problem vector of independent Gaussian noise. The amount of this noise for both problems was set to be

$$\frac{\|\varepsilon\|_2}{\|b\|_2} = 0.01.$$

We have computed the solutions for a large set of regularization parameters. For each of the pairs of regularization parameters the relative image error was computed: $\frac{\|x - x^*\|_2^2}{\|x^*\|_2^2}$, where x^* is the ground truth image. The L-curves described in Section 3 are plotted

- in Figure 2 for the binary phantom for data fitting term and approximation of the class fitting term,

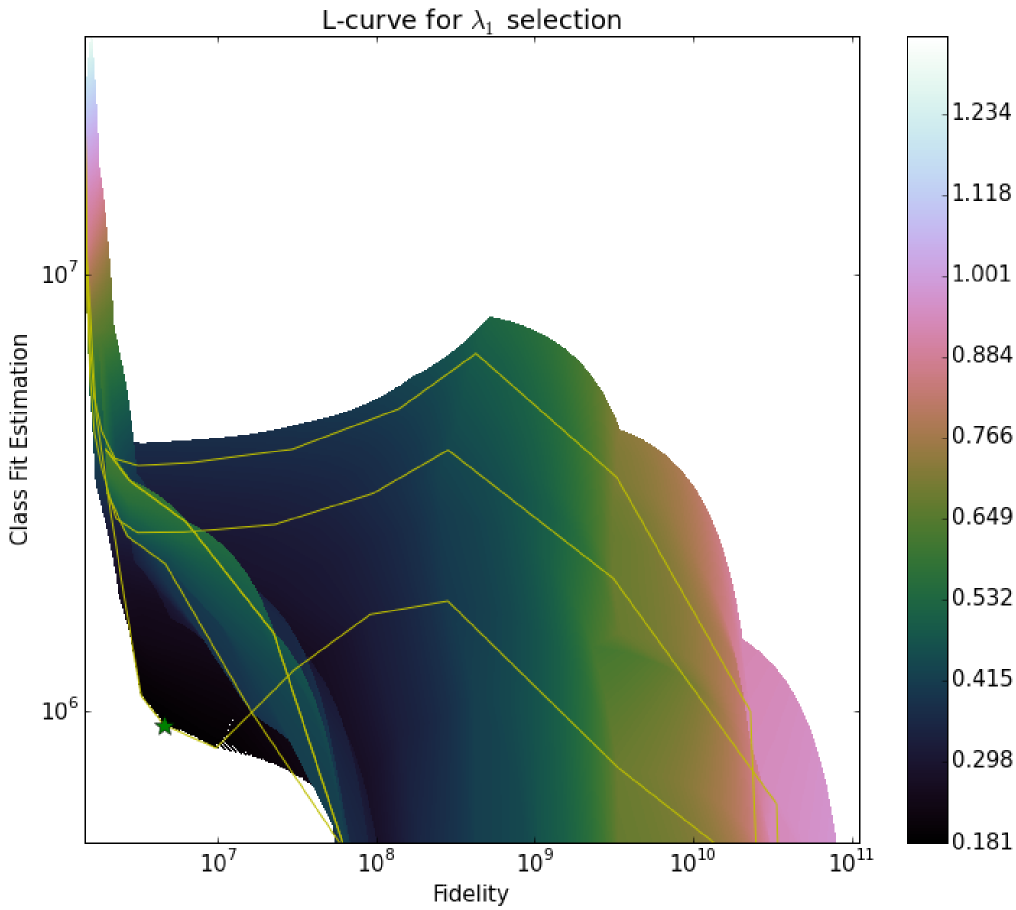

Figure 2: The modified L-curves plot for the Binary phantom for λ_1 parameter selection. The λ_2 parameter is constant along the yellow lines. The optimal pair of λ_1 and λ_2 parameters is denoted by a green star. The colour represents the relative image error in this point: $\frac{\|x-x^*\|_2^2}{\|x^*\|_2^2}$, where x^* is the ground truth, x is the reconstructed image.

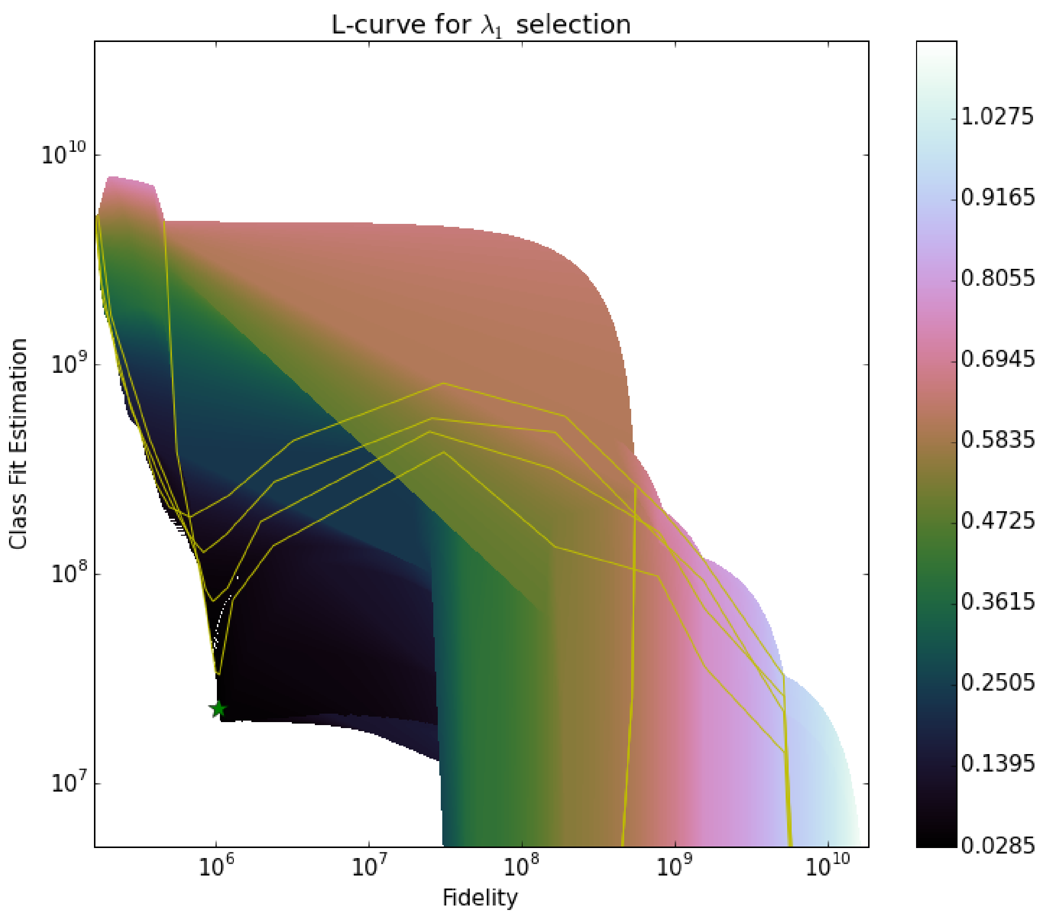

Figure 3: The modified L-curves plot for the Shepp-Logan phantom for λ_1 parameter selection. The λ_2 parameter is constant along the yellow lines. The optimal pair of λ_1 and λ_2 parameters is denoted by a green star. The colour represents the relative image error in this point: $\frac{\|x-x^*\|_2^2}{\|x^*\|_2^2}$, where x^* is the ground truth, x is the reconstructed image.

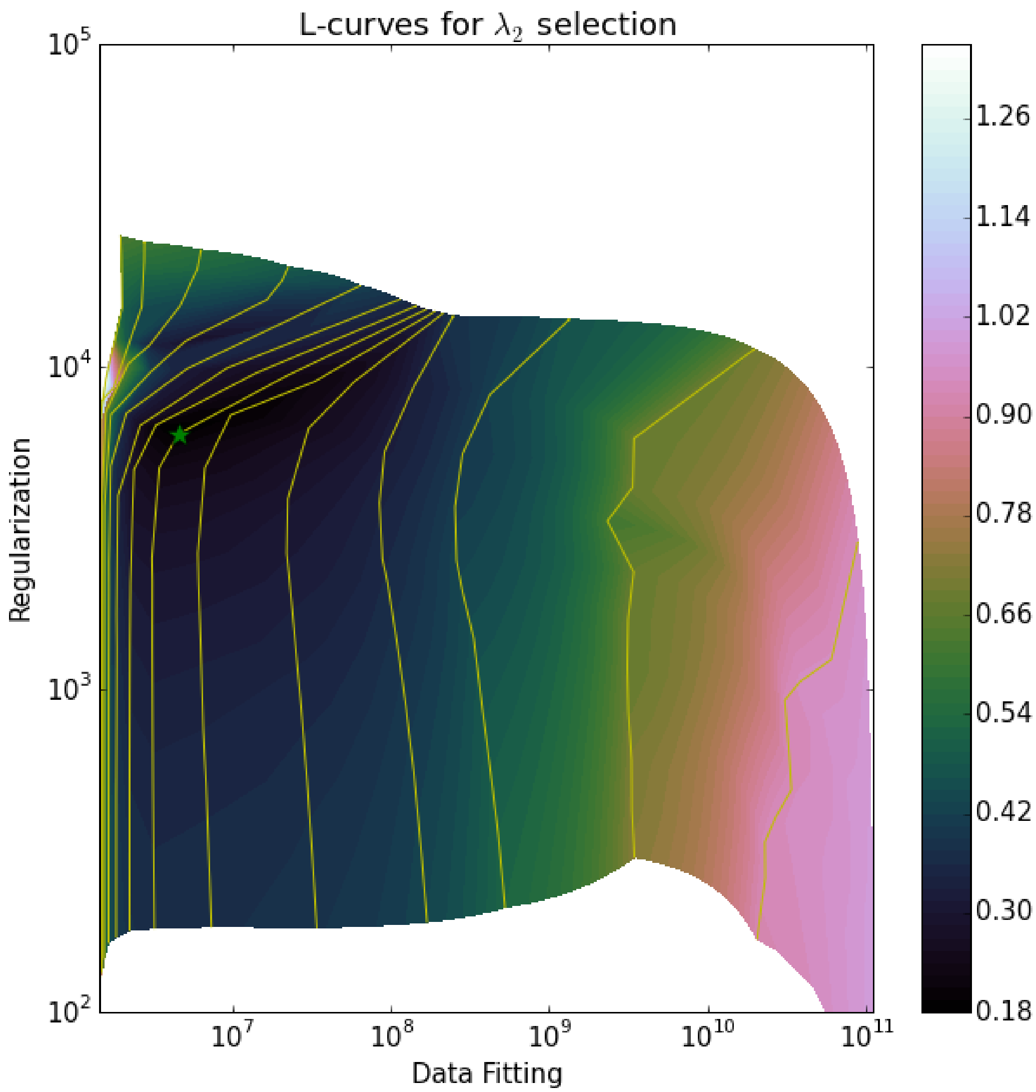

Figure 4: The modified L-curves plot for the Binary phantom for λ_2 parameter selection. The λ_1 parameter is constant along the yellow lines. The optimal pair of λ_1 and λ_2 parameters is denoted by a big green star. The colour represents the relative image error in this point: $\frac{\|x-x^*\|_2^2}{\|x^*\|_2^2}$, where x^* is the ground truth, x is the reconstructed image.

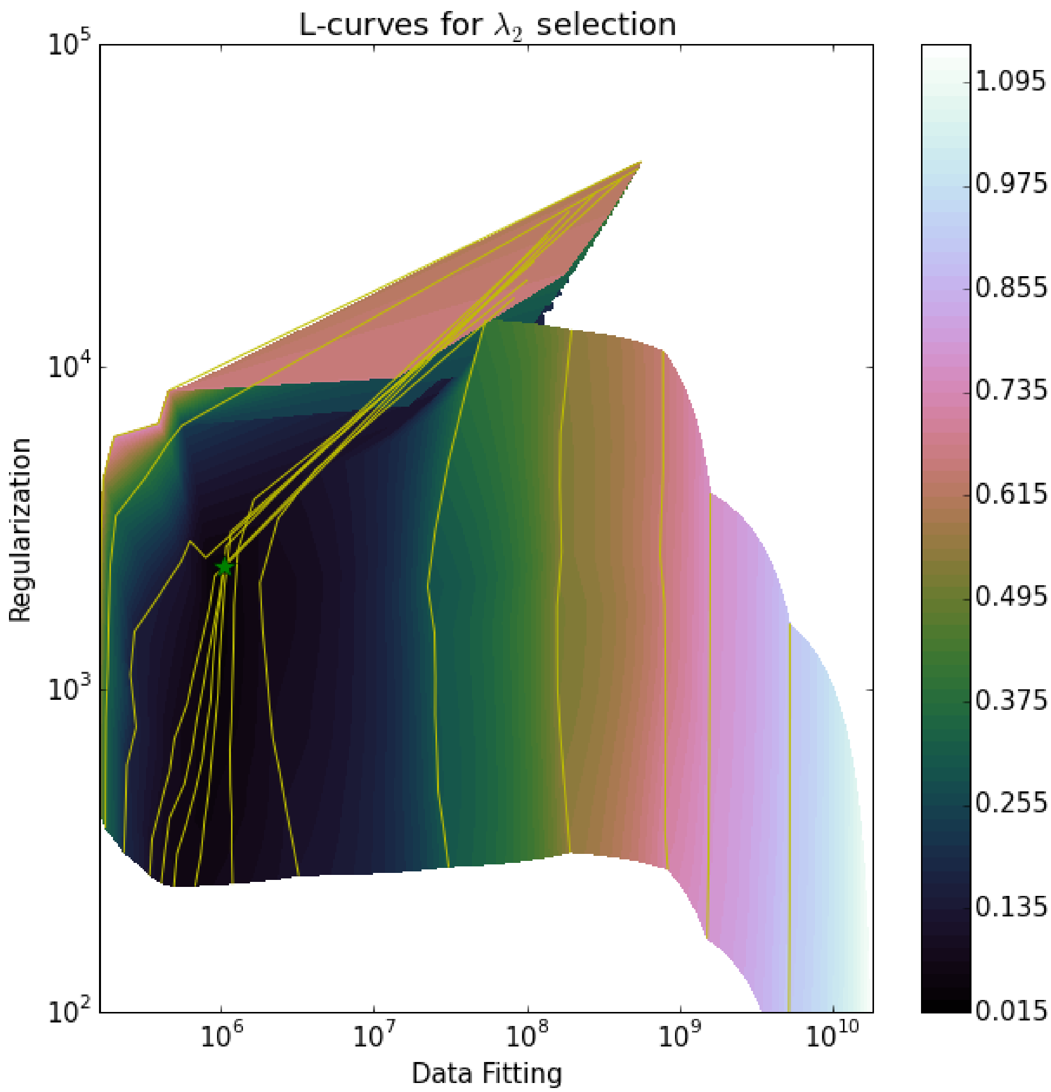

Figure 5: The modified L-curves plot for the Binary phantom for λ_2 parameter selection. The λ_1 parameter is constant along the yellow lines. The optimal pair of λ_1 and λ_2 parameters is denoted by a big green star. The colour represents the relative image error in this point: $\frac{\|x-x^*\|_2^2}{\|x^*\|_2^2}$, where x^* is the ground truth, x is the reconstructed image.

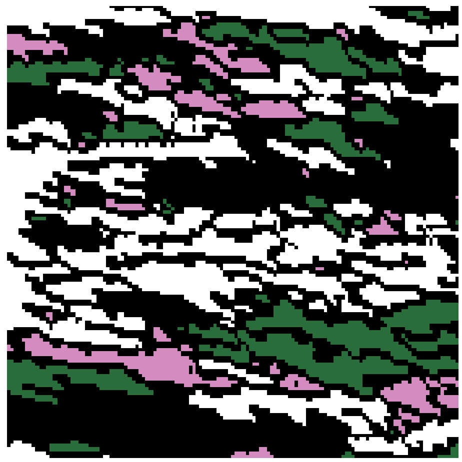

Figure 6: 4 class phantom for testing the L-curve approach testing.

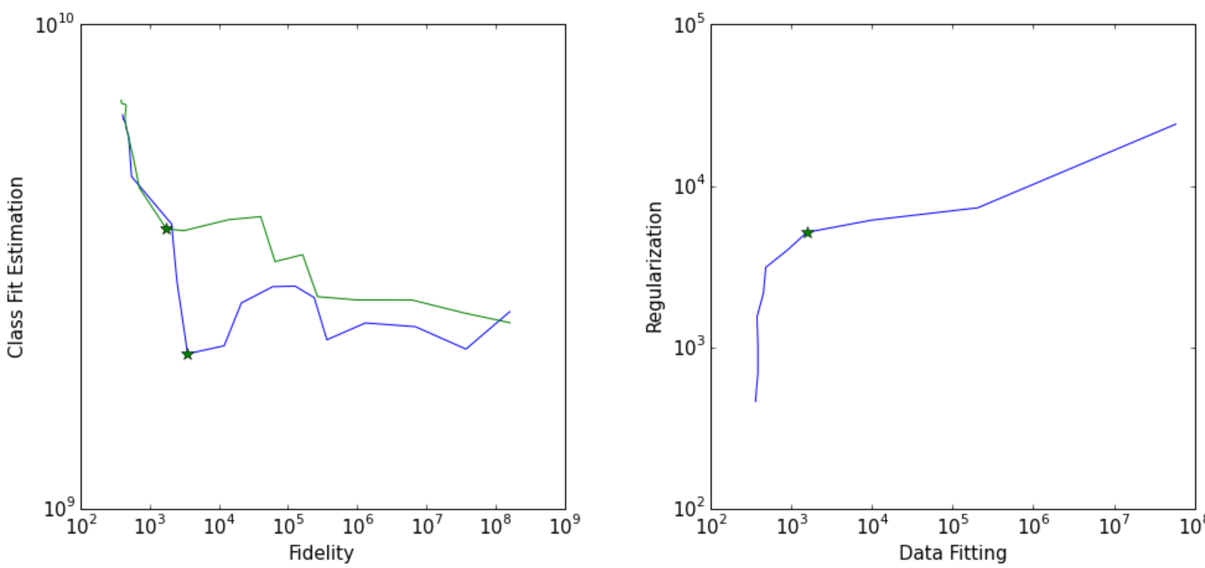

Figure 7: Testing of the regularization parameter selection approach. Left - curves for λ_1 parameter selection, blue - curve that corresponds to $\lambda_2 = 0.6$, green - curve that corresponds to $\lambda_1 = 0.78$, right - curve for λ_2 parameter selection. The green stars show the selected regularization parameters.

- in Figure 3 for the Shepp-Logan phantom for data fitting term and approximation of the class fitting term,
- in Figure 4 for the binary phantom for data fitting term and HMMFM regularization term,
- in Figure 5 for the Shepp-Logan phantom for data fitting term and HMMFM regularization term.

Consider the Figures 2 and 3. On these figures the yellow lines denote the lines, along which we do not change the λ_2 parameter changing only λ_1 regularization. Although these curves may look different, they have the shape that resembles the shape of the L-curve. Some of these lines have a corner. Also, we may note that the error value in the vicinity of the points where the L-curves change the behaviour is the smallest in all the figure (the error is denoted by a color). Thus, we may conclude that the regularization parameters that correspond to points in the vicinity of the corner of the L-curve produce good reconstruction. Thus, using this modified L-curves approach it is possible to select the λ_1 regularization parameter.

Next, consider the Figures 4 and 5. On these figures we do not change the λ_1 regularization parameter, changing only λ_2. We can see that the behaviour of these lines is different. We can see that the curves go from the left bottom corner up to the right top corner. In the beginning the curves go more or less along the axis. At some point the curve changes behaviour. We can see that the area where this happens corresponds to the optimal λ_2 regularization parameter. Thus, we have to find the λ_2 regularization parameter that corresponds to the point where the L-curve changes behaviour.

Using these approaches it is possible to find good regularization parameters λ_1 and λ_2 for the problem (6).

We have tested this approach on a test problem that contains 4 classes. The parameters of this problem are the same as the parameters of the problems considered above: the amount of the rays in the projection, the amount of projections, the amount of noise in the data, the geometry of projections are exactly the same. The attenuation coefficients that are present in the image are 0.0, 0.33, 0.66, 1.0. The phantom may be found on Figure 6

Next, consider the graphs in Figure 7. We have started with finding the λ_1 regularization parameter with $\lambda_2 = 0.6$. The λ_1 was selected to be equal to 1.83. After that, having the λ_1 regularization fixed, the λ_2 regularization was selected according to the rule that was stated above. The regularization parameter was selected to $\lambda_2 = 0.78$. Next, the search for the regularization parameter λ_1 was run again. The selected regularization parameter was again equal to 1.83. Thus, we have found the pair of regularization parameters: $\lambda_1 = 1.83, \lambda_2 = 0.78$. The relative image error that was achieved with these parameters is equal to 0.16.

5 Conclusion

We have shown that an L-curve approach to the problem of selection good regularization parameters with some modifications gives some ideas about how to select good regularization parameters for the SRS algorithm. Although the problem of finding good regularization parameters for our algorithm is very complicated due to non-convexity of the problem (6), the minimal modifications based on intuitive understanding is a good heuristic in this case. We have validated this approach with two artificial problems. Although to select the second regularization parameter λ_2 we cannot use the L-curve criterion itself, there is a convinient substitution for this criterion that we have formulated above.

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